MICROWAVE SPECTRA OF 9-FLUORENONE AND BENZOPHENONE

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The pure rotational spectra of 9-fluorenone ($C_{13}H_8O$) and benzophenone ($C_{13}H_{10}O$) were observed using chirped-pulse Fourier transform microwave spectroscopy (cp-FTMW). The 9-fluorenone spectrum was collected between 8 and 13 GHz, which allowed for the assignment of 124 rotational transitions. A separate spectrum spanning from 8 to 14 GHz was collected for benzophenone, allowing for the assignment of 133 rotational transitions. Both aromatic ketones exhibited strong b-type spectra with little to no centrifugal distortion, indicating highly rigid molecular structures. A comparison of the experimentally determined spectral constants of 9-fluorenone to those calculated using both ab initio and density functional theory strongly suggest the molecule conforms to a planar C_{2v} symmetric geometry as expected for its polycyclic structure. Whereas, a comparison of the experimental benzophenone constants to those predicted by theory suggests a molecule with non-planar C_2 symmetry, where the two phenyl groups are rotated approximately 32° out-of-plane to form a paddlewheel like geometry.